6 Software Programs to Increase the Utility of Predictive Microbiology Information*

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6.1 INTRODUCTION

The advent of computer technology and associated advances in computational power have made it possible to perform complex mathematical calculations that otherwise would be too time-consuming for useful applications in predictive microbiology. Computer software programs provide an interface between the underlying mathematics and the user, allowing model inputs to be entered and estimates to be observed through simplified graphical outputs. Examples of model software packages that

* Mention of brand or firm names does not constitute an endorsement by the U.S. Department of Agriculture over others of a similar nature not mentioned.

have gained wide use in the food industry and research communities include the Pathogen Modeling Program (PMP)* and the Food MicroModel (FMM).

Behind predictive software programs are the raw data upon which the models are built. Access to these data has become important for validating the robustness of models, for bringing transparency to microbial risk assessment, and for advancing modeling techniques. Recent initiatives, such as the relational database, *ComBase*, developed by the UK Institute of Food Research, Norwich, and US Department of Agriculture-Agricultural Research Service are compiling tens of thousands of predictive microbiology data sets to describe the growth, survival, and inactivation of microorganisms, and to accelerate model development and validation. Software databases and spreadsheets have made it possible to organize large quantities of data, and to search and retrieve specific items of information.

Along with advancements in databases and microbial modeling, a growing need has developed for decision-support tools for navigating across large quantities of data and retrieving specific information. Such information management systems have been used in other scientific fields, but have not been adequately developed and applied to predictive microbiology.

In this chapter, we present an overview of the role of commonly used software applications in the field of predictive microbiology, and we provide examples of software use in model interfaces, relational databases, and expert systems. Continued development and application of software programs in this field will improve the tools that are available to researchers and risk managers for enhancing the safety and quality of the food supply.

6.2 MODEL INTERFACES

Software programs have markedly enhanced the use of microbial models by the food industry, risk assessors, and food microbiologists. Well-designed interfaces with intuitive features allow users to define parameter inputs and then easily observe model outputs in graphic formats. This section describes more widely used predictive microbiology software with demonstrated applications in food safety and quality.

6.2.1 PATHOGEN MODELING PROGRAM

The PMP is a free software package of microbial models that describes growth, survival, inactivation, and toxin production under various conditions defined by the user (Buchanan, 1993). The current version, 6.1, contains 37 models for 10 bacterial pathogens that predict their growth and thermal and nonthermal inactivation. In addition, the PMP contains dynamic temperature models for the growth of *Clostridium perfringens* and *Clostridium botulinum.* Such dynamic models are increasingly sought by food industries that must meet performance standards for cooked–cooled meat products. Depending on the specific model, environmental variable inputs include atmosphere (aerobic or anaerobic), temperature (°F or °C), pH, water activity,

* U.S. Department of Agriculture-Agricultural Research Service *Pathogen Modeling Program* (www.arserrc.gov/mfs/pathogen.htm).

ionizing radiation, varying concentrations of lactic acid, sodium chloride, nitrite, and sodium pyrophosphate, or all of these. Model outputs for lag phase duration, generation time, and time to a user-defined level of interest are displayed in either hours or days. In addition, growth/inactivation curves are displayed in both graphical and tabular formats, along with associated upper and lower confidence limits. New features in the 6.1 version include links between specific models and associated publications, separate printing of output tables and figures, and input of time–temperature data sets in comma-separated-variable (csv) format. Future versions of the PMP will include direct links to the data sets underlying individual models, optional outputs for lag and no-lag scenarios, and operating the PMP on-line using Microsoft.Net database technology.

Similar to studies found in the scientific literature, the majority of the PMP 6.1 models were developed in defined microbiological media. Consequently, the PMP informs the user that there can be no guarantee that the predicted values will match those that would occur in a specific food system. To make the PMP models more useful to the food industry, as well as to food microbiologists and risk assessors, more food-specific models are under development. Examples of PMP 6.1 models include dynamic temperature for *C. perfringens* in cured beef and cured chicken (Juneja et al., 2001; Juneja and Marks, 2002), and growth models for *Salmonella typhimurium* on chicken breast meat (Oscar, 1999) with inputs for previous growth at variable temperatures and NaCl concentrations.

For the majority of the PMP models, bacterial growth and survival are represented by the Gompertz model. Although this approach is normally satisfactory for simple sigmoidal curves, the Gompertz model lacks the desired flexibility for modeling dynamic conditions that are relevant to commercial food production, particularly for thermally processed food. To meet this demand, future versions of the PMP will incorporate the dynamic model described by Baranyi and Roberts (1994).

6.2.2 Seafood Spoilage Predictor

The Seafood Spoilage Predictor* (SSP), produced by the Danish Institute of Fisheries Research, is a predictive microbiology software package for the microbial spoilage of fisheries products. It is more versatile than other similar programs by being able to predict food spoilage with both fixed and fluctuating temperatures. Also, the SSP has two model forms, relative rate of spoilage and microbial spoilage, which estimate spoilage as a function of organoleptic change and change in microbial levels, respectively.

6.2.3 Initiatives Leading to ComBase

The UK Institute of Food Research has produced curve-fitting softwares** that are increasingly used by researchers to develop predictive models. The PC-based Microfit and DMFit programs both use the model described by Baranyi and Roberts (1994) to fit curves to time versus colony-forming unit bacterial growth data. Microfit

* Danish Institute of Fisheries Research (http://www.dfu.min.dk/micro/ssp/).
** Institute of Food Research (www.ifr.bbsrc.ac.uk).

allows the user to compare the specific growth rates of different bacterial growth curves and to measure statistical significance. The DMFit program is an Excel®-based add-in feature that provides different types of curve-fitting programs and it plots the fit and the data for each data set. The DMFit software is an advantageous tool when the user anticipates incorporating the data sets into the ComBase relational database (described in the next section) because of similar data input formats.

The Food MicroModel (FMM)* was a commercial package of models with a graphical user interface, similar to the PMP (McClure et al., 1994); however, it has been discontinued in its original form. The FMM received extensive use by the food industry and offered users simple formats for inputting parameter values and obtaining model output data. It contained microbiological broth and food-specific models for pathogens and spoilage bacteria. Because of the commercial nature of the FMM, the user had limited access to its underlying models and data sets. Recently, the data behind the software have been merged with those that were generated for the PMP as well as data from international collaborators and from the published literature. The combined database (ComBase) is freely available at http://wyndmoor.arserrc.gov/combase/. The intention is to combine data and predictions in a unified Web-based database and model package called ComBase-PMP.

6.3 DATABASES

Predictive microbiology software packages are based on two main pillars: databases and mathematical models, and the scientific study of these belongs to both Bioinformatics and Biomathematics. Most chapters of this book deal with mathematical models; however, the present chapter is primarily dedicated to the other two members of this triangle (Figure 6.1).

The mutual dependence between mathematical models and databases is also confirmed by the fact that the ultimate tests for predictions are comparisons with observations. This can be done quickly and efficiently on large amounts of data only if the data-recording format is strictly standardized and harmonized with the respective mathematical variables.

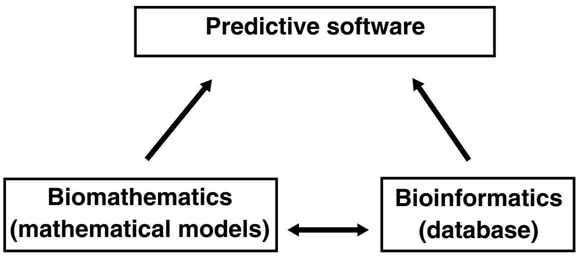


FIGURE 6.1 Relationship between predictive software, biomathematics, and bioinformatics.

* Leatherhead Food Research Association, UK (www.leatherheadfood.com/lfi/index.htm).

A database is a large collection of data organized especially for rapid search and retrieval. As an example, a typical, everyday-used database is a personal address book. Its computer form can be conceived as a table of rows and columns, where the rows and columns are termed *records* and *fields*, respectively. In an address book, typical fields are the name, address, and phone number. Fields belonging together (in our example, belonging to one person) form a record.

When defining the fields, one must define the "resolution" of the database according to the tasks for which it is used. A field, such as the address in our example, could be further divided into town and street, thus increasing the resolution of the record. However, this may cause problems when such an address as "Oak House, Kingston" is to be recorded, with no street name. Therefore, if there is no special reason for further resolution, it is unnecessary to subdivide the field. A valid reason for further refinement could be if it was a frequent task to list those persons who live on the same street.

Similar problems are encountered when building a database on microbial responses to the environment. For the benefit of a fast data search, those elements of information that are likely to be searched should be recorded in specified fields, in a specified format. Therefore, the first step when building such a database is to define the fields and their syntax, i.e., what values can be in a field. Typically, these values are either numeric (for quantities) or alphabetic (for categories). It is common to provide an interval for the values found in the numeric fields; similarly a list of values can be used to define the content of a category field.

Because of the complexity of the food environment and the tedious nature of food microbiology measurements, predictive food microbiology is typically a scientific field where well-organized databases are in high demand. For example:

1. The inaccuracy of measurements can be compensated by numerous measurements.
2. The variability of responses is a main focus of investigation, and quantification and modeling of variability require replicate measurements.
3. International data exchange cannot be done without defining compatible database formats.

Accordingly, the first question when building a database is: What to record? In this respect, the construction of a database is similar to that of a mathematical model; both are, in some way, the art of omitting the unnecessary. One cannot record all available information on microbiology experiments; some simplification and categorization is inevitable. The way these simplifications are carried out is sometimes arguable, even subjective, but undoubtedly necessary, just as mathematical models are necessarily simplified descriptions of nature, to understand and predict complex phenomena. The distribution of information among database categories (fields) is parallel to assigning mathematical variables to certain quantities; the relationship between those fields, for fast search and interrogation, is parallel to relationships and equations between mathematical variables for deriving conclusions and predictions in a mathematical way.

In general, producing software of microbiology data commonly involves the following stages of development:

Level 1 — Raw data: these are as recorded by the person generating the data, usually in spreadsheet format.
Level 2 — Database: these are sets of data, systematically categorized and recorded, following a predefined structure (syntax). To create a database, one needs computational skill, understanding of the data, and the ability to make expert judgments when necessary.
Level 3 — Browser: a computer program to navigate in the database.
Level 4 — Simple predictions: these are usually interpolated values given by mathematical equations, for example, the FMM or the PMP is at this level.
Level 5 — Complex predictions (dynamic conditions, growth/no growth boundary, probability of growth, Bayesian methods, expert systems): at the moment, no predictive software package is available at level 5.

A new predictive microbiology initiative called ComBase is described by Baranyi and Tamplin (2002). It aims at pooling data in a common database for predictive microbiology purposes. The database will be a source of publicly available information on bacterial responses to food environments.

One of the most important features of ComBase is that it can record not only a single value in a field but also a "pointer" to a table, representing the variable changing with time. A dynamic profile can be recorded this way, as a list of (time, value) pairs, for either an environmental factor or a response variable. ComBase is available via the Internet.

6.4 EXPERT SYSTEMS

The increased use of computer technology in food production, the widespread use of the Internet in business, and the increasing ease and speed of development of user-friendly software opens up a number of possibilities for software solutions in supporting decisions that are based on predictive microbiology. This section describes a number of ways in which decision-support software can contribute. We focus on the employment of a particular class of software programs called expert systems. These tools formally encapsulate knowledge and data and, given input through a user-interface, generate conclusions and analyses to inform the user.

6.4.1 Types of Computer-Based Decision Support

The simplest way in which computers can support decisions is to provide for intelligent storage and retrieval of data. This storage and retrieval can be easily extended to add documentation retrieval. More advanced decision-support systems can perform complex calculations given user input and then present results in appropriate formats.

Beyond data storage, data retrieval and the implementation of calculations is a class of tools that can bring a higher level of functionality and knowledge to decision

support (Level 5 described above). These tools can bring more domain-specific knowledge to the decision-support function by including more complex knowledge, relationships among pieces of knowledge, and can impose a knowledge-based structure on the decision process.

Earlier in this chapter we discussed large predictive microbiology databases (e.g., ComBase) and model interfaces (e.g., PMP) that are derived from these data. Decision-support tools can be used to navigate across vast quantities of predictive microbiology information, retrieve specific information, and then to build and validate microbial models. Furthermore, decision-support tools can potentially direct the user to alternative sources of information when appropriate models and data are lacking.

An example of more complex decision support is the use of expert systems. While a number of software tools whose functionality is derived from expert knowledge may be called *expert systems*, the term is most appropriately applied to software that provides advisory information based on a set of rules and algorithms for inference based on the relationships underlying these rules.

In these systems, the core knowledge is stored as a series of IF–THEN rules that connect diverse evidence such as user input, data from databases, and the formalized opinions of experts into a web of knowledge. Software tools are available to facilitate the development of these rule-based systems, including tools to handle the user interface and creation of an executable, stand-alone software product. Recently, the capacity to create Internet-ready expert systems has been developed and integrated into these development tools to greatly facilitate the dissemination of expert knowledge in terms of both the development time and the ease of its delivery to users.

There are various examples of decision-support systems which encapsulate knowledge that is based in predictive microbiology. Examples include decision-support tools to be applied in predicting food safety and shelf life (Wijtes et al., 1998; Zwietering et al., 1992), and a step-wise system structured as a standard risk assessment process to assist in decisions regarding microbiological food safety (van Gerwen et al., 2000). Other examples of decision-support systems for microbial processes are described by Voyer and McKellar (1993) and Schellekens et al. (1994).

Expert systems provide two main forms of decision support. They impose a structure on the inference such that there is a consistent and deterministic pathway between user input, data, and conclusions. This is useful where the decision domain benefits from the assurance of consistency and where there is a desire to remove more subjective elements of decision-making from the overall decision process. For organizations dealing with recurring and complex food safety issues, consistency and reliability of decision-making may provide assurance to buyers, regulators, and the organization itself that safety will not be compromised by unstructured or ill-informed decision-making. In addition to concerns for subjective and variable decision-making, the proper structuring of the decision (in terms of delineating and weighing the necessary considerations and accessing the required knowledge to support the decision) may itself be the most difficult task for nonexpert users to carry out.

A second form of decision support provided by expert systems is to capture and make available the expert knowledge itself. The result of the conversion of expert

knowledge into a set of rules that can generate advice in the absence of direct expert interaction could be a valuable asset for many institutions. Such tools may be particularly useful when provided to smaller organizations that do not have ready access to scientific expertise. The expertise that may be held by relatively few persons can be made available to many users who might otherwise compete for the attention of a few experts. In addition, time spent addressing repetitive enquiries can detract from the expert's own efforts in maintaining and enhancing his knowledge base, thus diminishing the overall generation of knowledge in an organization. With respect to food safety, a key ingredient in the process is the knowledge and decision processes that must be applied to assure a safe product. An expert system could provide assurance of the supply and the quality of this knowledge ingredient.

6.4.2 Possible Applications of Expert Systems

A number of possibilities exist for the development of decision-support systems based on rule-based expert systems. Examples (Paoli, 2001) include:

Virtual inspection: Simulating interaction with an inspector to allow establishments to self-assess their facility or a food processing operation. This may be of interest to large companies and regulators who find their quality control or inspection resources inadequate for the number of establishments that they are required to assess.

Process deviation assessment: Tools which incorporate expert knowledge regarding the best actions to take in case of process deviations, in terms of assessing the seriousness of the deviation and in recommending corrective actions for the implicated product and the process.

Problem-oriented education: Apart from providing expert advice, an expert system could be used to assist in education regarding the importance of key variables and to foster careful reasoning among operational decision-makers.

In-line real-time expert systems: Examples exist (though not in predictive microbiology) of expert systems that receive real-time data and provide continuous assessments of the status of systems, based on the combination of these data and embedded knowledge-based rules that interpret the data for display to operators. This could be applied to food production systems where a complex set of variables requires monitoring combined with complex reasoning to assure safety and quality.

6.4.3 Application to Qualitative Risk Assessment

Of international interest may be applications in the area of qualitative risk assessment. While most of the recent attention in the field of microbiological risk assessment has been paid to quantitative risk assessment (see Chapter 8), there is increasing interest in the relative merits and drawbacks of a more qualitative form of risk assessment. The merits of such an approach include the speed with which such an analysis could be performed and the decreased reliance on quantitative data which is often unavailable. Some drawbacks include the potential for qualitative risk

assessment to become little more than a literature search with loose and unstructured reasoning and untraceable conclusions.

Currently, there are no formal guidelines specifying what type of analysis would constitute a properly performed qualitative risk assessment. Were such guidelines to be developed, an expert system could be produced which encapsulated and imposed an appropriate risk assessment process, as well as some of the requisite knowledge that would be required to assure an adequate qualitative risk assessment. Recent work by Crawford-Brown (2001) is an example of a decision-support tool to assist in the development of a highly structured and well-documented qualitative risk assessment. Further examples of this type of tool might be of great benefit to those who would like to capture the potential value of systematic risk assessment while avoiding the computational and data burden of quantitative approaches.

6.5 CONCLUSIONS

On the basis of the trends seen for the past ten years it can be said that the demand for predictive microbiology software programs will expand with increasing application of microbial models to food systems. This includes the use of predictive models for research and for the development of Hazard Analysis and Critical Control Points systems, product formulation, and risk assessment. Concomitantly, continued advances in database and decision-support software, as well as Internet technologies, will provide risk managers with better tools for seeking relevant information and making informed decisions. However, to sustain this effort, multiinstitutional collaborations will be critical for managing the input, organization, quality control, and dissemination of large quantities of predictive microbiology data. Ultimately, these advances will provide researchers, students, and educators with greater access to information for improving the safety and quality of the food supply.

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